

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 221 °C

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 4.87e-01

Nearest Neighbors from the Training Set

Image not found

Dichlorvos

Measured: 234

Predicted: 221

Image not found

Sulfurous acid, bis(2-methylpropyl) ester

Measured: 210

Predicted: 214

Image not found

Sulfurous acid, dibutyl ester

Measured: 230

Predicted: 226

Image not found

Phosphonothioic acid, methyl-, O,o-diethyl ester

Measured: 199

Predicted: 194

Image not found

Diethyl phosphorochloridate

Measured: 93.5

Predicted: 125